Supplementary Material for "Two-photon Absorption Properties of Gold Fluorescent Protein: A Combined Molecular Dynamics and Quantum Chemistry Study"

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Table S1: Atom name, atom type, coordinates and charges of 4IN residue in the topology.

No	Atom Name	Atom Type	x	y	z	Charge
1	N	N	36.950188	46.626678	51.645828	-0.982449
2	H	H	37.166000	47.348301	52.306656	0.404902
3	CA	CT	38.044861	46.488235	50.684772	0.247510
4	HA	H1	37.755760	46.769371	49.674267	0.025056
5	CB	CT	39.255032	47.338215	51.108860	-0.184328
6	HB2	HC	40.109303	46.928192	50.584461	0.094119
7	HB3	HC	39.434975	47.197746	52.169575	0.094119
8	CG	C*	39.124447	48.775070	50.811367	0.010949
9	CD1	CW	38.911652	49.779980	51.709099	-0.209523
10	HD1	H4	38.795002	49.727356	52.773434	0.217190
11	NE1	NA	38.871368	50.991428	51.062359	-0.366098
12	CE2	CN	39.062740	50.789856	49.719643	0.071695
13	CD2	CB	39.223392	49.404129	49.520500	0.077590
14	CE3	CA	39.431007	48.930836	48.215828	0.197608
15	N16	N2	39.597198	47.592651	47.904194	-0.765727
16	H161	H	39.540550	47.394115	46.928806	0.373318
17	H162	H	39.067661	46.932983	48.428082	0.373318
18	CZ3	CA	39.470726	49.853451	47.162163	-0.211702
19	HZ3	HA	39.640781	49.508663	46.157185	0.156865
20	CH2	CA	39.312016	51.223152	47.396381	-0.211134
21	CZ2	CA	39.107525	51.712055	48.666359	-0.192095
22	HZ2	HA	38.989876	52.762791	48.860619	0.148969
23	HH2	HA	39.351139	51.905052	46.564964	0.180342
24	HE1	H	38.802193	51.876991	51.504021	0.392900
25	C	C	38.483650	45.030956	50.505859	0.572927
26	O	O	38.758488	44.597504	49.388168	-0.516326

Table S2: Atom name, atom type, coordinates and charges of 5ZA residue in the topology.

No	Atom Name	Atom Type	x	y	z	Charge
1	N26	N	43.001553	42.454414	41.759941	-0.843244
2	H26	H	42.710114	42.267117	42.701214	0.377481
3	C22	CT	44.286674	41.668697	41.458038	0.204128
4	H22	H1	44.637764	42.002590	40.484989	0.089630
5	C23	CT	45.301483	42.035477	42.469345	0.273552
6	H23	H1	46.286541	41.867641	42.041485	-0.023710
7	C25	CT	45.186337	43.506050	42.875660	-0.084527
8	H251	HC	45.960167	43.742996	43.595333	0.030567
9	H252	HC	44.228977	43.707195	43.342625	0.030567
10	H253	HC	45.302921	44.159824	42.017632	0.030567
11	O24	OH	45.199780	41.447979	43.638752	-0.664456
12	H24	HO	45.329021	40.516293	43.498531	0.461930
13	C14	CK	43.732483	40.259892	41.359749	0.096987
14	N13	NB	43.861324	39.372738	42.272045	-0.362781
15	C12	CC	43.321918	38.205101	41.909767	-0.004337
16	C11	CD	43.223076	37.003407	42.632061	-0.045685
17	C7	C*	43.639687	36.760693	43.946812	-0.084334
18	C1	CB	43.518055	35.570919	44.698849	0.112322
19	C2	CA	43.030586	34.283779	44.523899	0.197600
20	N10	N2	42.421543	33.800556	43.245831	-0.769512
21	H101	H	42.159550	32.838375	43.285423	0.362871
22	H102	H	43.004845	33.947613	42.448250	0.362871
23	C3	CA	43.074928	33.310032	45.584736	-0.206643
24	H3	HA	42.700397	32.315010	45.419102	0.152422
25	C4	CA	43.616020	33.635509	46.836105	-0.200378
26	H4	HA	43.669979	32.911922	47.630638	0.174389
27	C5	CA	44.116257	34.931351	47.039375	-0.196619
28	H5	HA	44.510895	35.189720	48.005363	0.158536
29	C6	CN	44.064175	35.873432	45.981266	0.019584
30	N9	NA	44.485481	37.130829	46.002548	-0.292711
31	C8	CW	44.244656	37.685547	44.804855	-0.073250
32	H8	H4	44.502506	38.702244	44.609077	0.152733
33	H9	H	44.892647	37.602619	46.776928	0.365772
34	H11	HA	42.775238	36.180374	42.109196	0.127140
35	C16	C	42.813427	38.427162	40.592407	0.495710
36	O17	O	42.218147	37.589855	39.849560	-0.544364
37	N15	N*	43.066833	39.750973	40.292614	-0.031517
38	C18	CT	42.676983	40.491909	39.049789	0.011294
39	H182	H1	42.482445	41.520901	39.305546	0.063414
40	H183	H1	41.757378	40.026516	38.717186	0.063414
41	C19	C	43.646641	40.420021	37.951530	0.474157
42	O21	O	43.155613	40.596405	36.762833	-0.461572

Table S3: Force field parameters generated by PyRED(SEP-2015)[1] for 5ZA and 4IN residues.

MASS	mass	pol
C	12.010	0.616
C*	12.010	0.360
CA	12.010	0.360
CB	12.010	0.360
CC	12.010	0.360
CD	12.010	0.360
CN	12.010	0.360
CR	12.010	0.360
CT	12.010	0.878
CW	12.010	0.360
CX	12.010	0.360
H	1.008	0.161
H1	1.008	0.135
H4	1.008	0.167
HA	1.008	0.167
HC	1.008	0.135
HO	1.008	0.135
N*	14.010	0.530
N2	14.010	0.530
NA	14.010	0.530
NB	14.010	0.530
NT	14.010	0.530
O	16.000	0.434
OH	16.000	0.465

BOND	K($\frac{kcal}{mol \times ang^2}$)	Dist0(ang)
C – CT	315	1.522
C – CX	315	1.522
C – N*	425	1.383
C – O	570	1.229
C – OH	450	1.364
C* – CB	390	1.459
C* – CT	315	1.495
C* – CW	545	1.352
CA – CA	470	1.400
CA – CN	470	1.400
CA – HA	365	1.080
CB – CN	445	1.419
CC – NB	410	1.394
CD – HA	365	1.080
CN – NA	430	1.380

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CR – NB	490	1.335
CT – CT	310	1.526
CT – CX	310	1.526
CT – H1	340	1.090
CT – HC	340	1.090
CT – N*	335	1.475
CT – NT	365	1.471
CT – OH	320	1.410
CW – H4	365	1.080
CW – NA	425	1.381
CX – H1	340	1.090
H – N2	435	1.010
H – NA	435	1.010
H – NT	435	1.010
HO – OH	555	0.960
ANGLE	K($\frac{kcal}{mol \times rad^2}$)	Theta0(deg)
CT – C – O	80	120.4
CT – C – OH	80	110.0
CX – C – O	80	120.4
CX – C – OH	80	110.0
N* – C – O	80	120.9
O – C – OH	80	120.0
CB – C* – CT	70	128.6
CB – C* – CW	65	106.4
CT – C* – CW	70	125.0
CA – CA – CA	65	120.0
CA – CA – CN	65	120.0
CA – CA – HA	50	120.0
CN – CA – HA	50	120.0
C* – CB – CN	65	108.8
CA – CN – CB	65	122.7
CA – CN – NA	70	132.8
CB – CN – NA	70	104.4
C – CT – H1	50	109.5
C* – CT – CX	65	115.6
C* – CT – HC	50	109.5
CT – CT – CT	40	109.5
CT – CT – H1	50	109.5
CT – CT – HC	50	109.5
CT – CT – NT	80	111.2
CT – CT – OH	50	109.5
CX – CT – HC	50	109.5

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Table S3 – continued from previous page

H1 – CT – H1	35	109.5		
H1 – CT – N*	50	109.5		
H1 – CT – NT	50	109.5		
H1 – CT – OH	50	109.5		
HC – CT – HC	35	109.5		
C* – CW – H4	50	120.0		
C* – CW – NA	70	108.7		
H4 – CW – NA	50	120.0		
C – CX – CT	65	111.1		
C – CX – H1	50	109.5		
CT – CX – H1	50	109.5		
C – N* – CT	70	117.6		
H – N2 – H	35	120.0		
CN – NA – CW	70	111.6		
CN – NA – H	50	123.1		
CW – NA – H	50	120.0		
CC – NB – CR	70	117.0		
CT – NT – H	50	109.5		
H – NT – H	35	109.5		
C – OH – HO	50	113.0		
CT – OH – HO	55	108.5		
DIHEDRAL	Path	V($\frac{kcal}{mol \times rad}$)	Phase(deg.)	Period
O – C – CT – H1	1	0.800	0	-1
O – C – CT – H1	1	0.000	0	-2
O – C – CT – H1	1	0.080	180	3
O – C – CT – N*	1	0.000	0	2
OH – C – CT – H1	1	0.000	0	2
OH – C – CT – N*	1	0.000	0	2
O – C – CX – CT	1	0.000	0	2
O – C – CX – H1	1	0.800	0	-1
O – C – CX – H1	1	0.000	0	-2
O – C – CX – H1	1	0.080	180	3
O – C – CX – NT	1	0.000	0	2
OH – C – CX – CT	1	0.000	0	2
OH – C – CX – H1	1	0.000	0	2
OH – C – CX – NT	1	0.000	0	2
CC – C – N* – CR	1	1.450	180	2
CC – C – N* – CT	1	1.450	180	2
O – C – N* – CR	1	1.450	180	2
O – C – N* – CT	1	1.450	180	2
CT – C – OH – HO	1	2.300	180	2
CX – C – OH – HO	1	2.300	180	2

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Table S3 – continued from previous page

O – C – OH – HO	1	2.300	180	-2
O – C – OH – HO	1	1.900	0	1
CD – C* – CB – CD	1	1.680	180	2
CD – C* – CB – CN	1	1.680	180	2
CT – C* – CB – CD	1	1.680	180	2
CT – C* – CB – CN	1	1.680	180	2
CW – C* – CB – CD	1	1.680	180	2
CW – C* – CB – CN	1	1.680	180	2
CB – C* – CT – CX	1	0.000	0	2
CB – C* – CT – HC	1	0.000	0	2
CW – C* – CT – CX	1	0.000	0	2
CW – C* – CT – HC	1	0.000	0	2
CB – C* – CW – H4	1	6.530	180	2
CB – C* – CW – NA	1	6.530	180	2
CD – C* – CW – H4	1	6.530	180	2
CD – C* – CW – NA	1	6.530	180	2
CT – C* – CW – H4	1	6.530	180	2
CT – C* – CW – NA	1	6.530	180	2
CA – CA – CA – CD	1	3.630	180	2
CA – CA – CA – CN	1	3.630	180	2
CA – CA – CA – HA	1	3.630	180	2
CD – CA – CA – HA	1	3.630	180	2
CN – CA – CA – HA	1	3.630	180	2
HA – CA – CA – HA	1	3.630	180	2
CA – CA – CN – CB	1	3.630	180	2
CA – CA – CN – NA	1	3.630	180	2
HA – CA – CN – CB	1	3.630	180	2
HA – CA – CN – NA	1	3.630	180	2
C* – CB – CN – CA	1	3.000	180	2
C* – CB – CN – NA	1	3.000	180	2
CD – CB – CN – CA	1	3.000	180	2
CD – CB – CN – NA	1	3.000	180	2
C – CC – NB – CR	1	2.400	180	2
CD – CC – NB – CR	1	2.400	180	2
CA – CN – NA – CW	1	1.530	180	2
CA – CN – NA – H	1	1.530	180	2
CB – CN – NA – CW	1	1.530	180	2
CB – CN – NA – H	1	1.530	180	2
CT – CR – NB – CC	1	5.000	180	2
N* – CR – NB – CC	1	5.000	180	2
CR – CT – CT – CT	1	0.156	0	3
CR – CT – CT – H1	1	0.156	0	3
CR – CT – CT – OH	1	0.156	0	3

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CT – CT – CT – H1	1	0.156	0	3
CT – CT – CT – HC	1	0.160	0	3
CT – CT – CT – NT	1	0.156	0	3
H1 – CT – CT – H1	1	0.156	0	3
H1 – CT – CT – HC	1	0.156	0	3
H1 – CT – CT – NT	1	0.156	0	3
H1 – CT – CT – OH	1	0.000	0	-3
H1 – CT – CT – OH	1	0.250	0	1
HC – CT – CT – OH	1	0.000	0	-3
HC – CT – CT – OH	1	0.250	0	1
NT – CT – CT – OH	1	0.156	0	3
C* – CT – CX – C	1	0.156	0	3
C* – CT – CX – H1	1	0.156	0	3
C* – CT – CX – NT	1	0.156	0	3
HC – CT – CX – C	1	0.156	0	3
HC – CT – CX – H1	1	0.156	0	3
HC – CT – CX – NT	1	0.156	0	3
C – CT – N* – C	1	0.000	0	2
C – CT – N* – CR	1	0.000	0	2
H1 – CT – N* – C	1	0.000	0	2
H1 – CT – N* – CR	1	0.000	0	2
CR – CT – NT – H	1	0.300	0	3
CT – CT – NT – H	1	0.300	0	3
H1 – CT – NT – H	1	0.300	0	3
CT – CT – OH – HO	1	0.160	0	-3
CT – CT – OH – HO	1	0.250	0	1
H1 – CT – OH – HO	1	0.167	0	3
C* – CW – NA – CN	1	1.500	180	2
C* – CW – NA – H	1	1.500	180	2
H4 – CW – NA – CN	1	1.500	180	2
H4 – CW – NA – H	1	1.500	180	2

IMPROPER	V($\frac{kcal}{mol \times rad}$)	Phase(deg.)	Period
CC – N* – C – O	10.5	180	2
CT – O – C – OH	10.5	180	2
CX – O – C – OH	10.5	180	2
CB – CT – C* – CW	1.1	180	2
CA – CA – CA – HA	1.1	180	2
CA – CD – CA – HA	1.1	180	2
CA – CN – CA – HA	1.1	180	2
C* – H4 – CW – NA	1.1	180	2
CN – CW – NA – H	1.0	180	2

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NONBON	R*(ang)	Eps($\frac{kcal}{mol}$)
C	1.908	0.0860
C*	1.908	0.0860
CA	1.908	0.0860
CB	1.908	0.0860
CC	1.908	0.0860
CD	1.908	0.0860
CN	1.908	0.0860
CR	1.908	0.0860
CT	1.908	0.1094
CW	1.908	0.0860
CX	1.908	0.1094
H	0.600	0.0157
H1	1.387	0.0157
H4	1.409	0.0150
HA	1.459	0.0150
HC	1.487	0.0157
HO	0.000	0.0000
N*	1.824	0.1700
N2	1.824	0.1700
NA	1.824	0.1700
NB	1.824	0.1700
NT	1.824	0.1700
O	1.661	0.2100
OH	1.721	0.2104

Listing S 1: Amber parameters for minimization of the system with a 10 $kcal/mol/\text{Å}^2$ restraints.

```
minimization of all systems with restraints
&cntrl
imin     = 1
ntx      = 1
ntxo     = 2
ntpr     = 500
ntwx     = 500
ntf      = 1
ntb      = 1
cut      = 12
ntr      = 1
ntmin    = 1
maxcyc   = 10000
ncyc     = 5000
restraint_wt  = 10
restraintmask = ':1-225'
/
```

Listing S 2: Amber parameters for minimization of the system without restraints.

```
minimization of all systems without restraints
&cntrl
imin     = 1
ntx      = 1
ntxo     = 2
ntpr     = 500
ntwx     = 500
ntf      = 1
ntb      = 1
cut      = 12
ntr      = 0
ntmin    = 1
maxcyc   = 5000
ncyc     = 2500
/
```

Listing S 3: Amber parameters for heating the system from 0K to 300K with a 10 $kcal/mol/\text{Å}^2$ restraints.

```
Heating of protein from 0K to 300K with restraints
&cntrl
imin     = 0
irest    = 0
ntx      = 1
ntb      = 1
ntxo     = 1
cut      = 12
ntr      = 1
ntc      = 2
ntf      = 2
tempi    = 0.0
temp0    = 300.0
ntt      = 3
gamma_ln= 1.0
nstlim   = 100000
dt       = 0.002
ntpr     = 500
ntwx     = 500
ntwr     = 500
restraint_wt     = 10
restraintmask    =':1-225'
/
```

Listing S 4: Amber parameters for equilibration at 300K with a 1 $kcal/mol/\text{Å}^2$ restraints.

```
Equilibration at 300K with a restraints
&cntrl
imin         = 0
irest    = 1
ntx      = 5
ntb      = 2
ntxo     = 1
cut      = 12
ntr      = 1
ntc      = 2
ntf      = 2
tempi    = 300.0
temp0    = 300.0
ntt      = 3
ntp      = 1
```

```
pres0   = 1.0
taup    = 2.0
gamma_ln= 1.0
nstlim  = 1000000
dt      = 0.002
ntpr    = 500
ntwx    = 500
ntwr    = 500
restraint_wt    = 1
restraintmask   =':1-225'
/
```

Listing S 5: Amber parameters for production simulation of the system.

```
Molecular dynamics at 300K
&cntrl
imin    = 0
irest   = 1
ntx     = 5
ntb     = 2
ntxo    = 1
cut     = 12
ntp     = 1
pres0   = 1.0
taup    = 2.0
igb     = 0
nscm    = 10000
ioutfm  = 1
ntc     = 2
ntf     = 2
tempi   = 300.0
temp0   = 300.0
ntt     = 3
gamma_ln= 1.0
nstlim  = 5000000
dt      = 0.002
ntpr    = 100
ntwx    = 1
ntwr    = 500
/
```

Listing S 6: GAMESS-US Parameters for TPA calculations.

```
$SYSTEM
   PARALL=.T.
   MEMORY=530000000   ! 4.043 GB
$END
!------ CONTROL ----------------------------------------#
$CONTRL
   UNITS=ANGS
   ISPHER=-1
   MOLPLT=.T.
   PLTORB=.T.
   MAXIT=200
   ICHARG=0
   MULT=1
   RUNTYP=ENERGY
   EXETYP=RUN
   SCFTYP=RHF
   DFTTYP=CAMB3LYP
   TDDFT=EXCITE
   NPRINT=7
$END
!------ BASIS SET DEFINITION ----------------------------#
$BASIS
   GBASIS=N31
   NGAUSS=6
   DIFFSP=.T.
   DIFFS=.T.
   NDFUNC=1
$END
!------ SELF-CONSISTENT FIELD CONTROLS ------------------#
$SCF
   DIIS=.T.
   SOSCF=.F.
   NOCONV=.F.
   DAMP=.T.
   SHIFT=.T.
   NPREO(1)=0,-1,1,9999
$END
!------ TD-DFT ------------------------------------------#
$TDDFT
   NSTATE=1
   IROOT=1
   MULT=1
   TPA=.T.
```

```
   TAMMD=.F.
 $END
 !------ Initial molecular orbitals ----------------------#
 $GUESS
   GUESS=HUCKEL
 $END

 $DATA

C1
H       1.0       44.070829       41.246485       41.339720
C       6.0       43.761959       40.212505       41.383129
N       7.0       43.946602       39.369820       42.333675
C       6.0       43.379436       38.202675       41.835197
C       6.0       43.196304       37.024372       42.532875
C       6.0       43.779499       36.782818       43.817307
C       6.0       43.147636       35.852539       44.737782
C       6.0       42.174377       34.781288       44.802727
N       7.0       41.448624       34.385666       43.732327
H       1.0       40.936230       33.520542       43.827770
H       1.0       41.492584       34.837902       42.830299
C       6.0       41.934391       34.090279       45.983337
H       1.0       41.139614       33.362206       46.051445
C       6.0       42.743301       34.214005       47.086594
H       1.0       42.506279       33.723217       48.018982
C       6.0       43.788319       35.173328       47.089157
H       1.0       44.416393       35.243721       47.964924
C       6.0       43.970379       36.008053       45.961143
N       7.0       44.899593       36.966877       45.667843
C       6.0       44.792564       37.438160       44.354797
H       1.0       45.310165       38.273865       43.907486
H       1.0       45.643776       37.241726       46.292946
H       1.0       42.504101       36.317860       42.099178
C       6.0       42.921360       38.334320       40.543358
O       8.0       42.214016       37.539692       39.849865
N       7.0       43.064232       39.673119       40.336456
H       1.0       42.786431       40.111681       39.458453
 $END
```

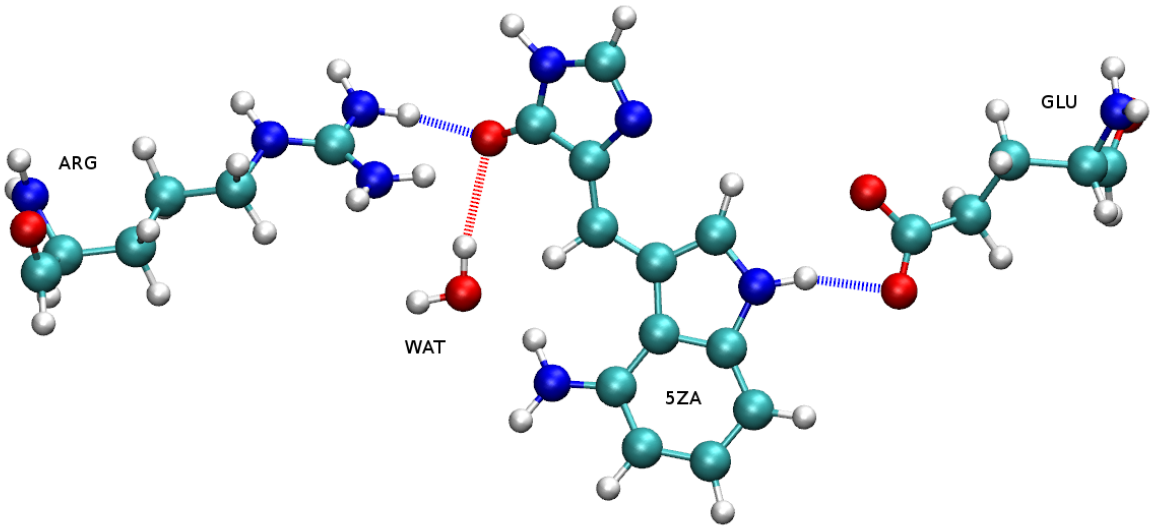

Figure S1: An example of Hydrogen bonding of 5ZA residue and surrounding water and residues via VMD[2] H bonding plugin.

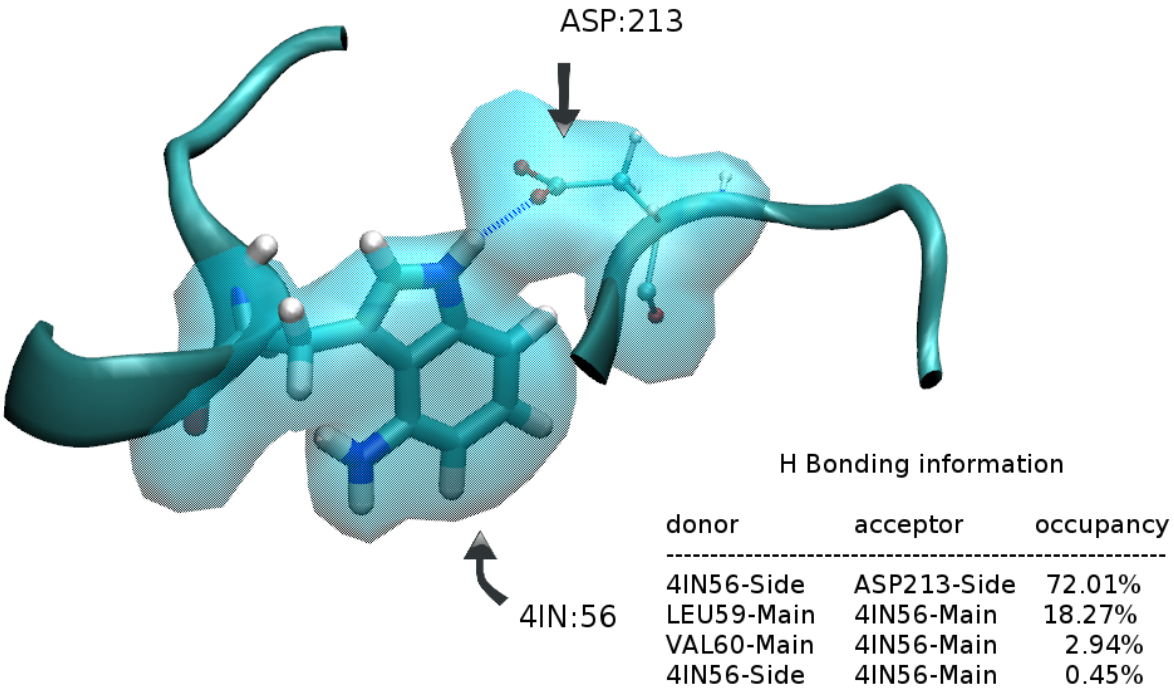

Figure S2: Hydrogen bonding analysis of 4IN residue with surrounding via VMD H bonding plugin. Surface representation shows the volume map of the 4IN:56 and ASP:213 residues, which make more H bondings over the simulation.

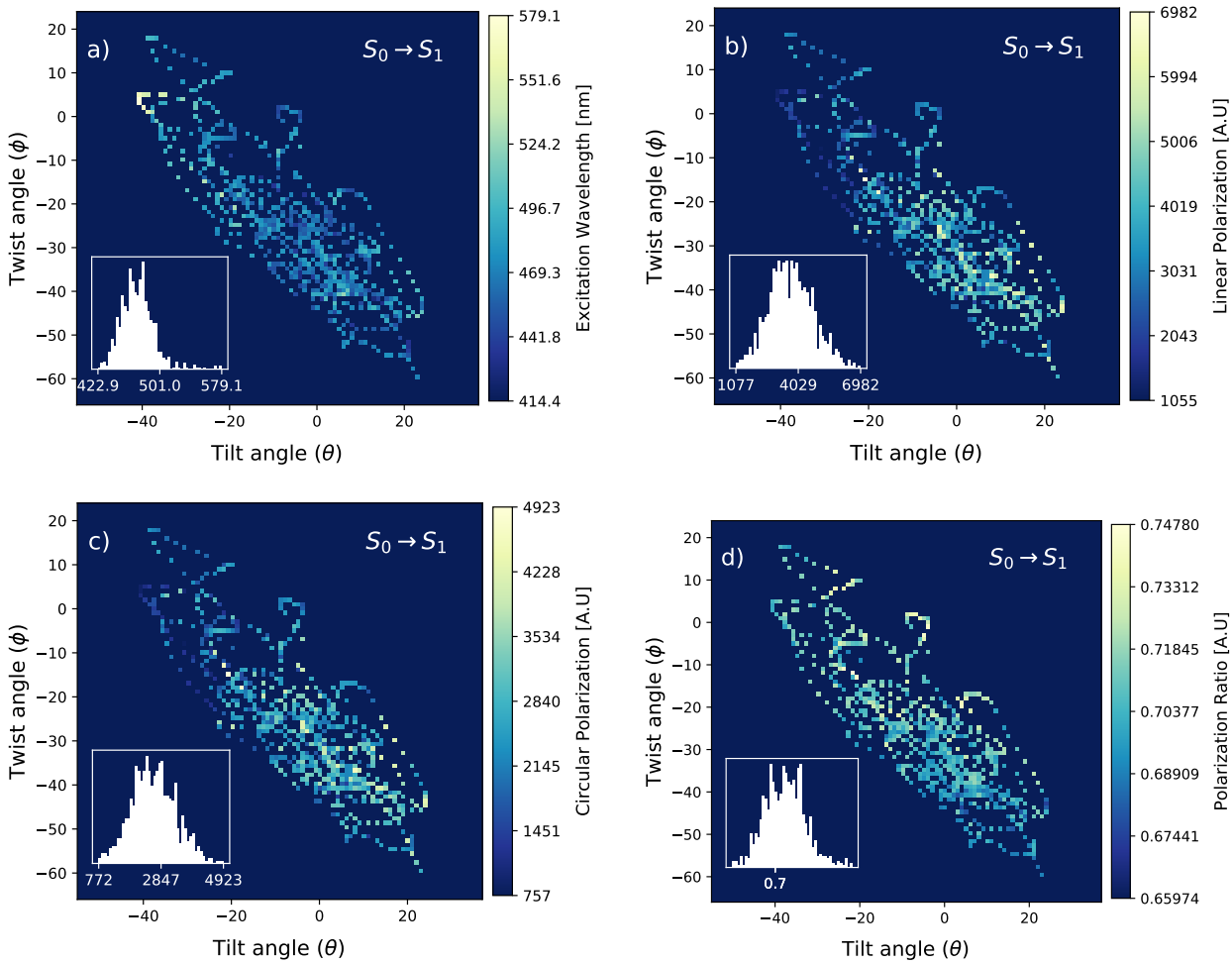

Figure S3: a) Excitation wavelength, b) Linear polarization, c) Circular polarization and d) Polarization ratios.

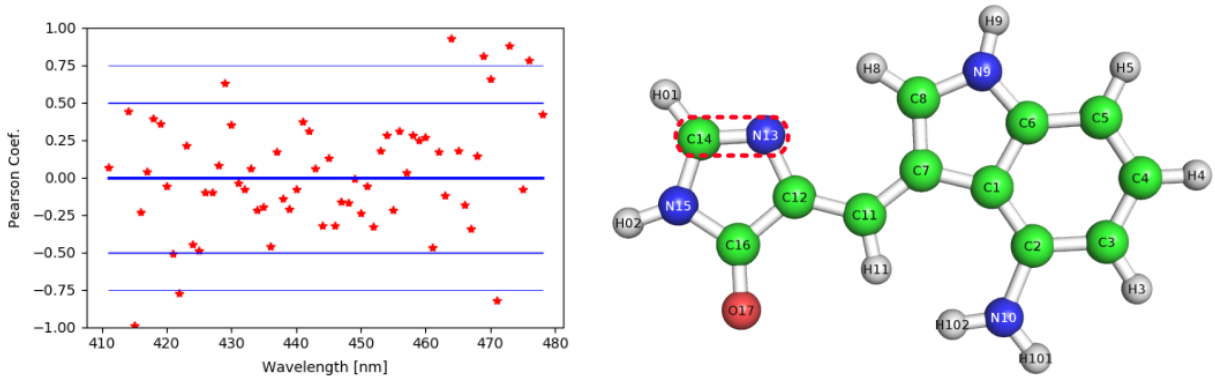

Figure S4: Pearson correlation analysis of bond "C14–N13".

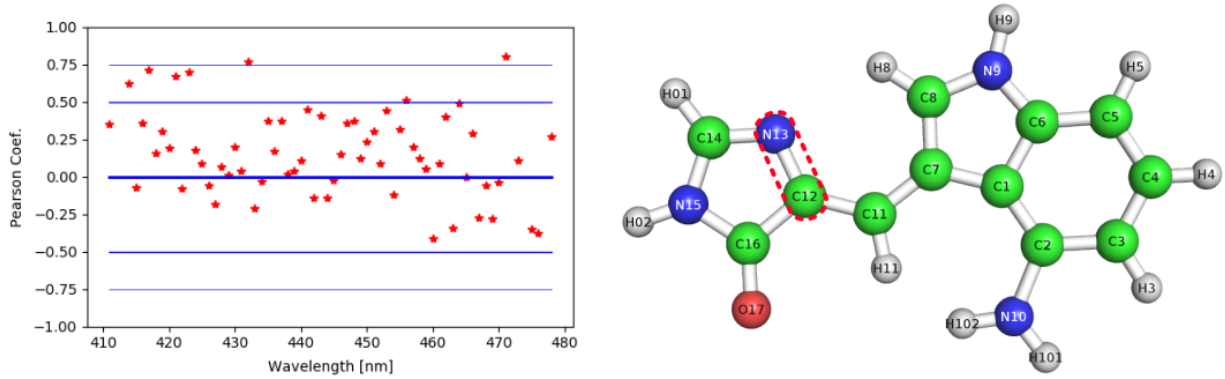

Figure S4 (cont.): Pearson correlation analysis of bond "N13–C12".

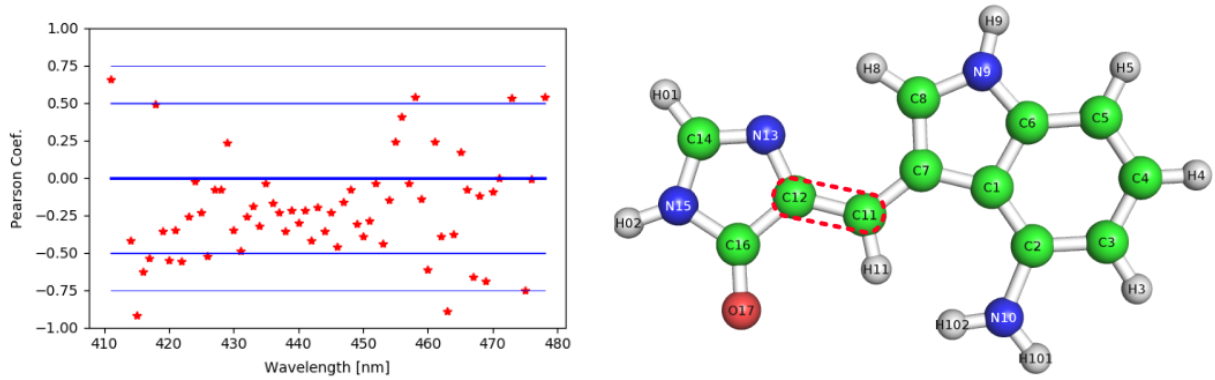

Figure S4 (cont.): Pearson correlation analysis of bond "C12–C11".

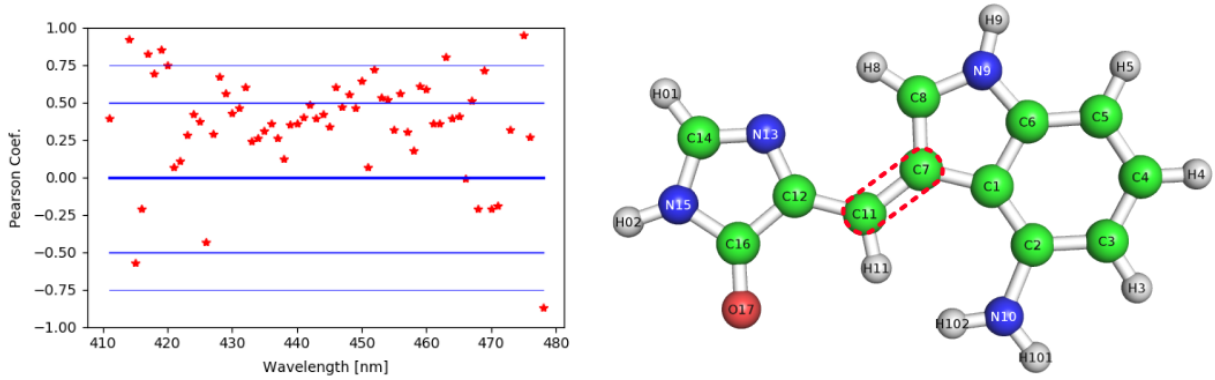

Figure S4 (cont.): Pearson correlation analysis of bond "C11–C7".

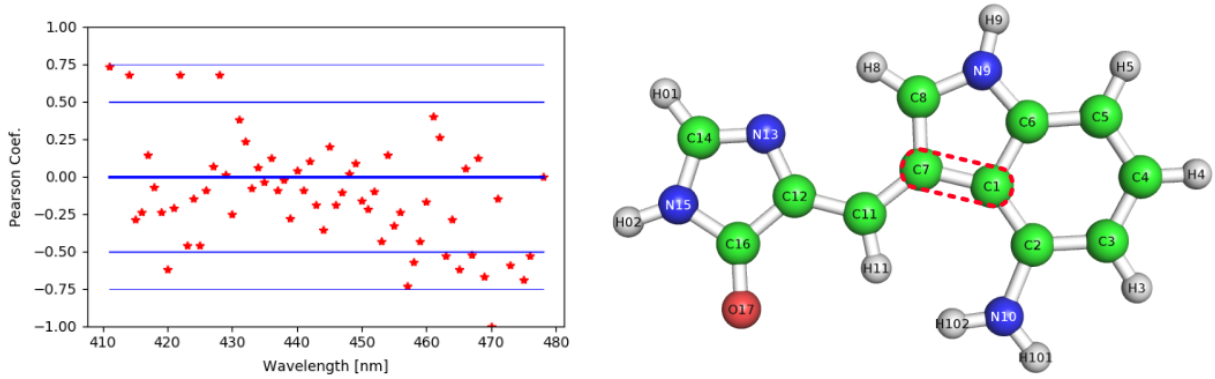

Figure S4 (cont.): Pearson correlation analysis of bond "C7–C1".

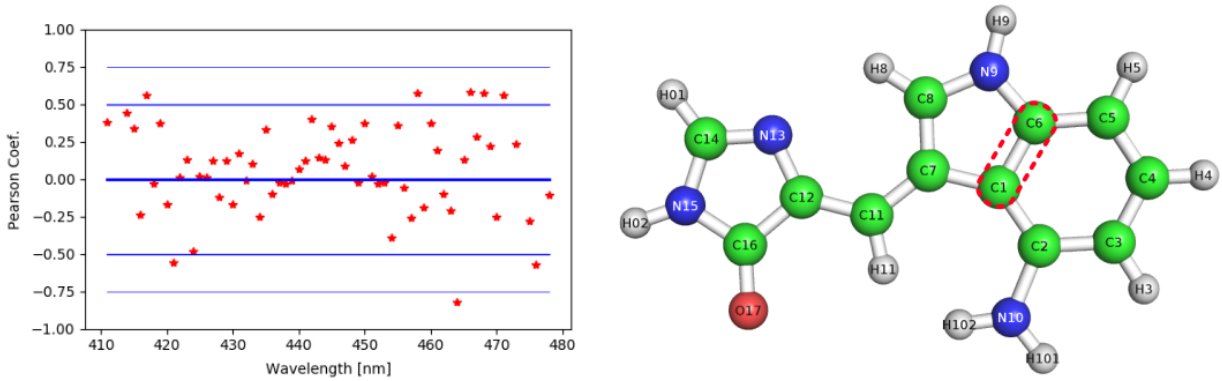

Figure S4 (cont.): Pearson correlation analysis of bond "C1–C6".

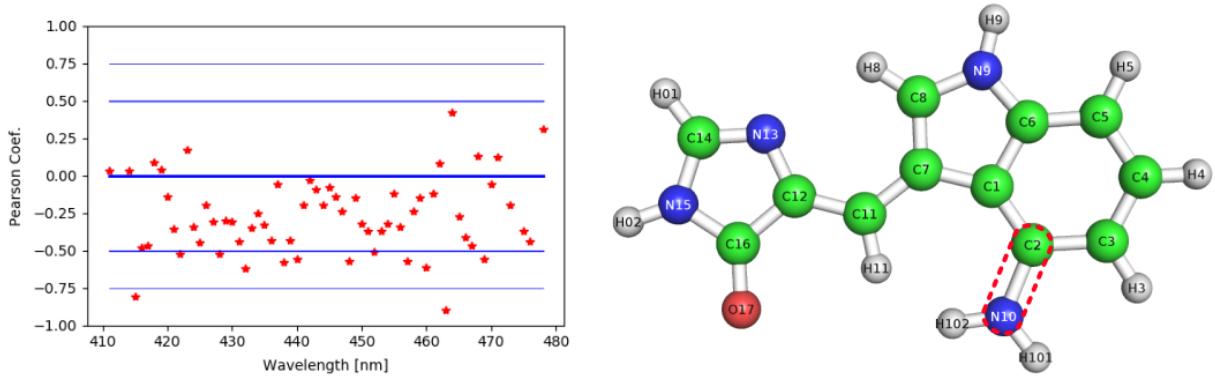

Figure S4 (cont.): Pearson correlation analysis of bond "C2–N10".

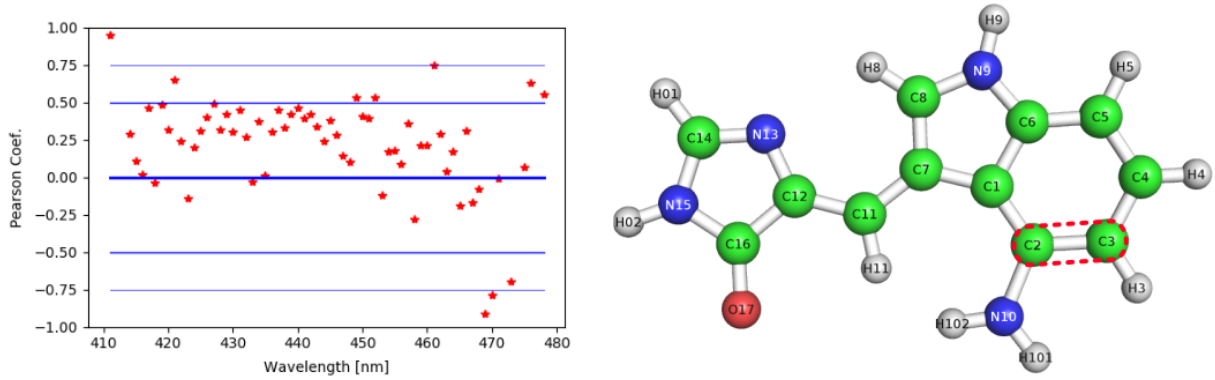

Figure S4 (cont.): Pearson correlation analysis of bond "C2–C3".

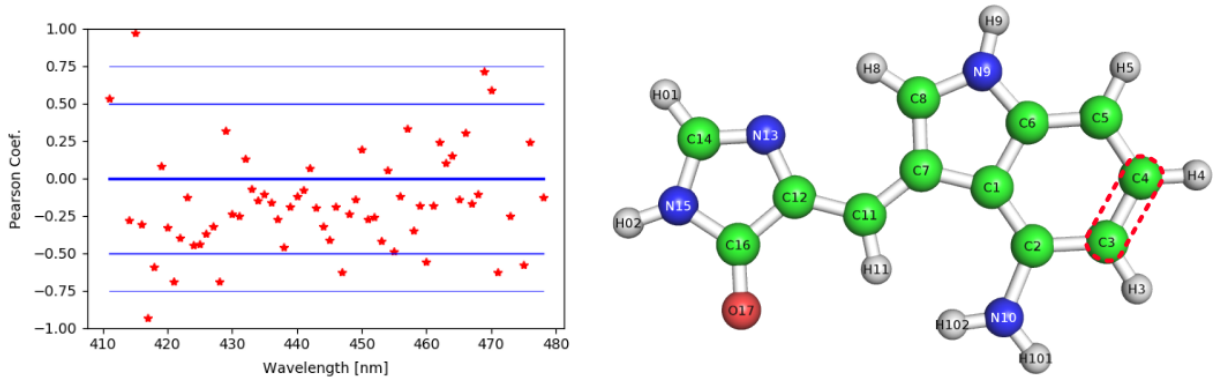

Figure S4 (cont.): Pearson correlation analysis of bond "C3–C4".

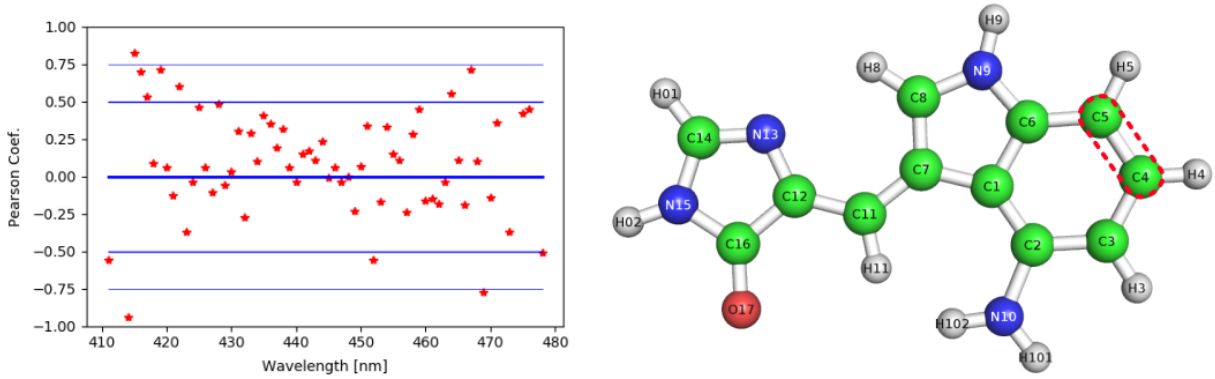

Figure S4 (cont.): Pearson correlation analysis of bond "C4–C5".

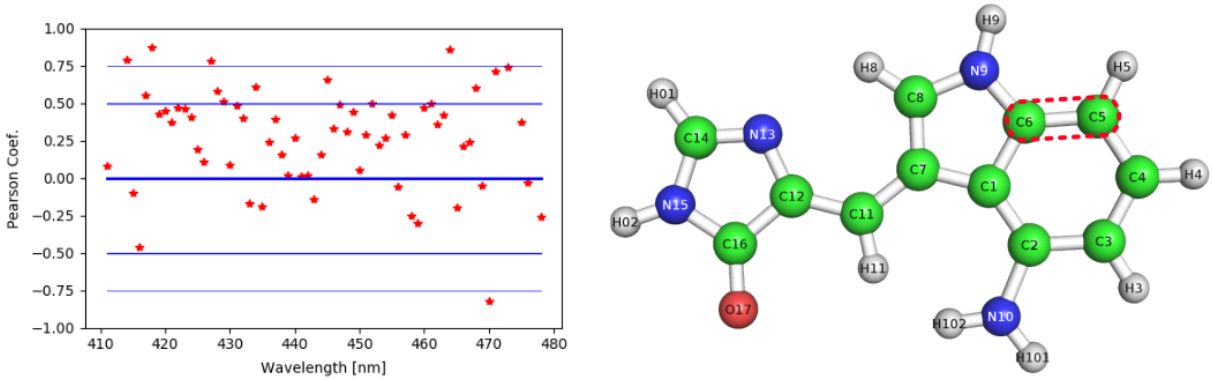

Figure S4 (cont.): Pearson correlation analysis of bond "C5–C6".

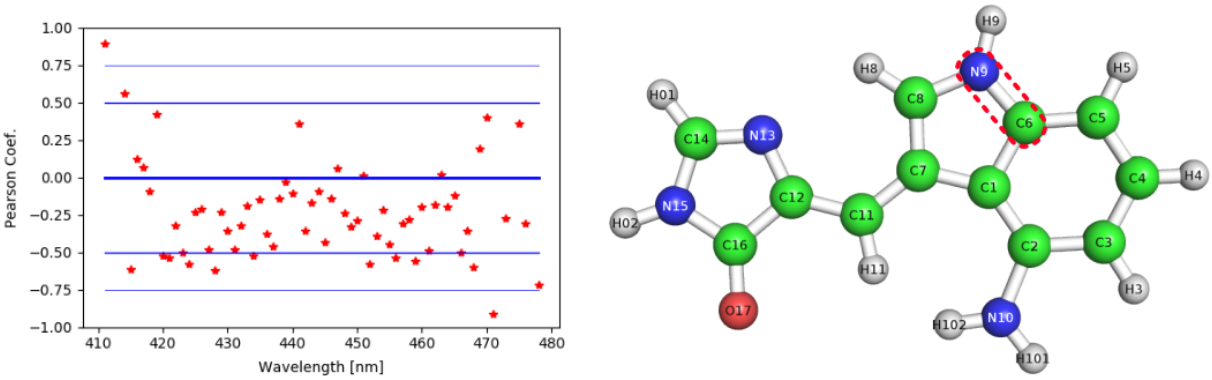

Figure S4 (cont.): Pearson correlation analysis of bond "C6–N9".

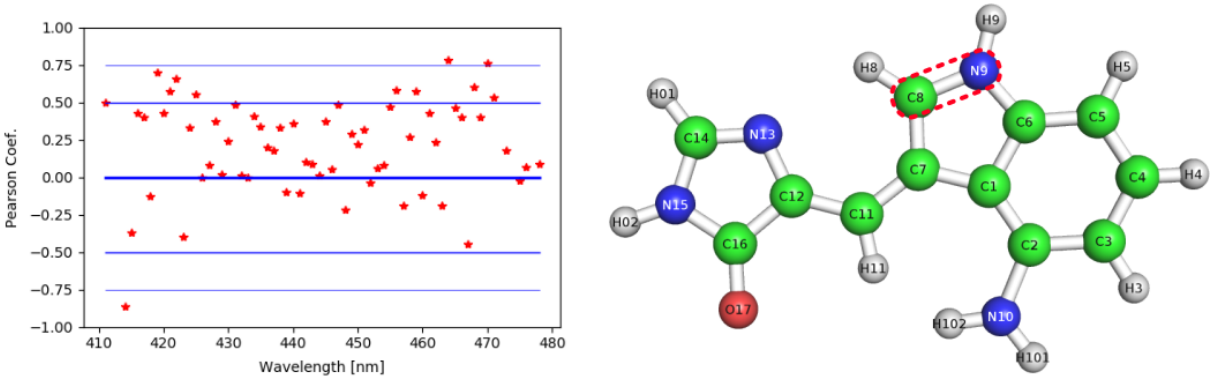

Figure S4 (cont.): Pearson correlation analysis of bond "C8–N9".

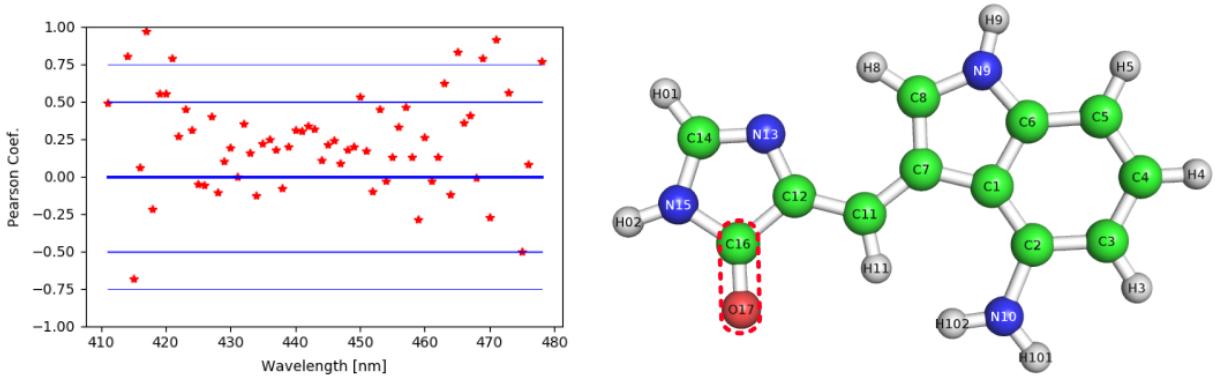

Figure S4 (cont.): Pearson correlation analysis of bond "C16–O17".

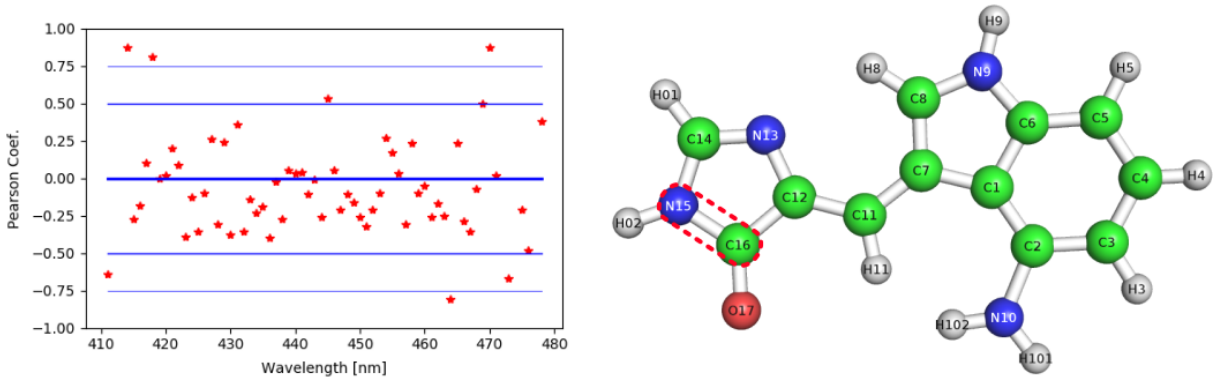

Figure S4 (cont.): Pearson correlation analysis of bond "C16–N15".

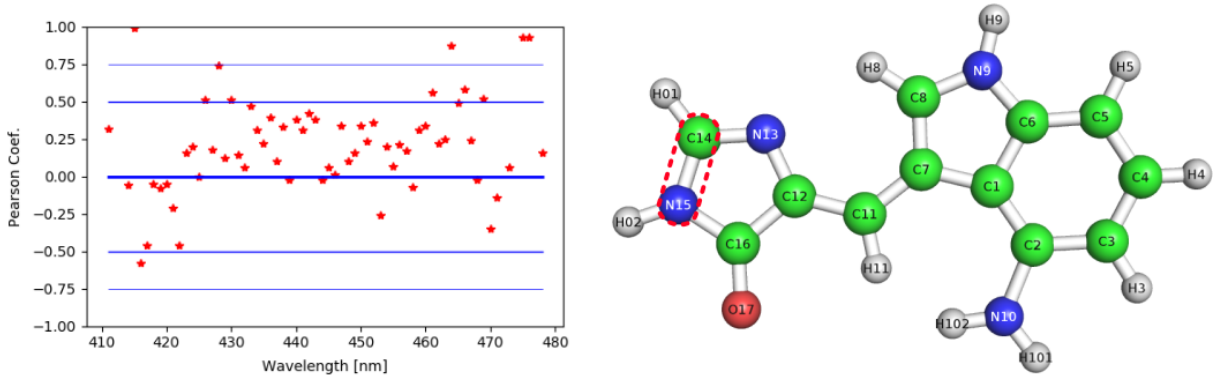

Figure S4 (cont.): Pearson correlation analysis of bond "C14–N15".

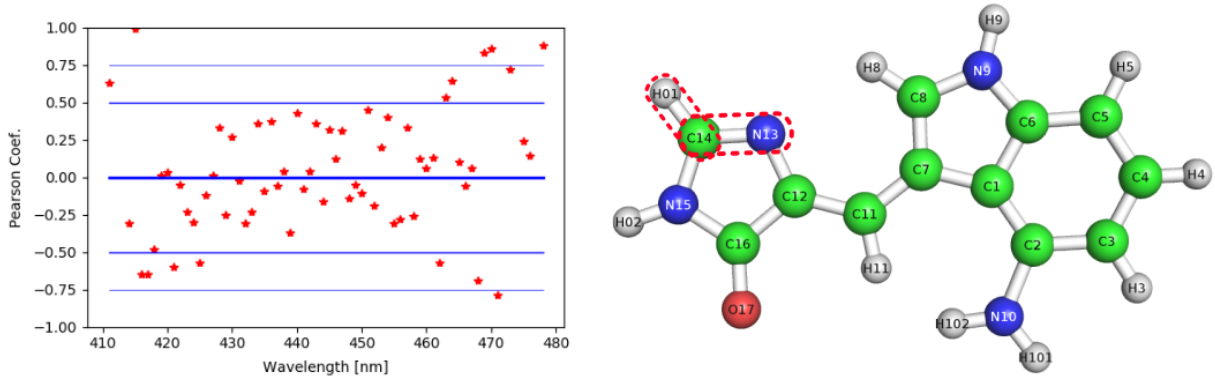

Figure S5: Pearson correlation analysis of angle "H01–C14–N13".

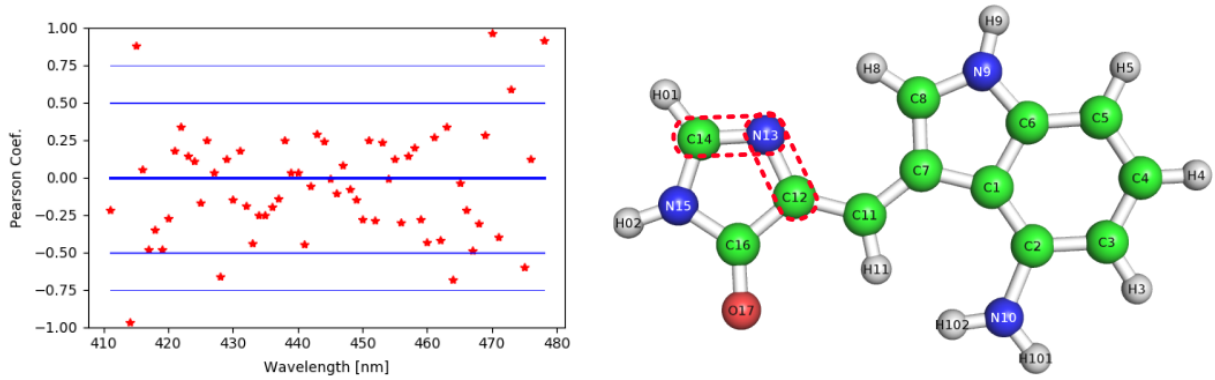

Figure S5 (cont.): Pearson correlation analysis of angle "C14–N13–C12".

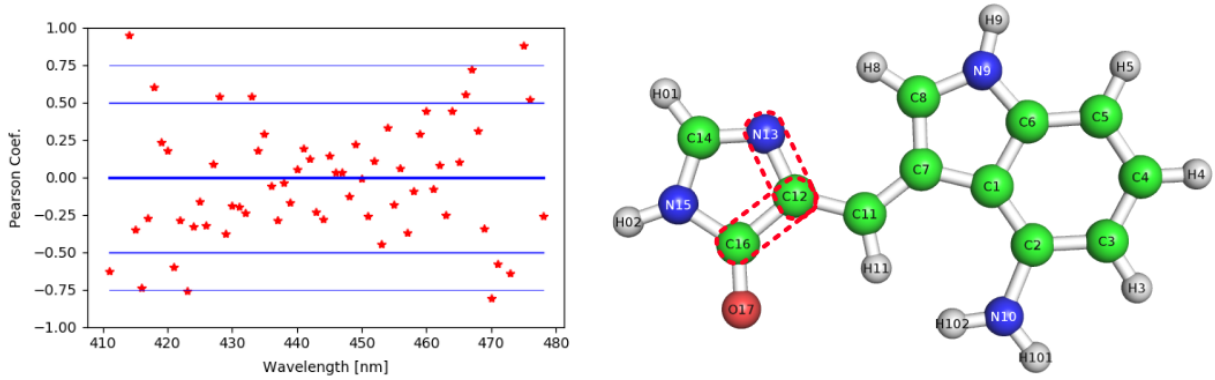

Figure S5 (cont.): Pearson correlation analysis of angle "N13–C12–C16".

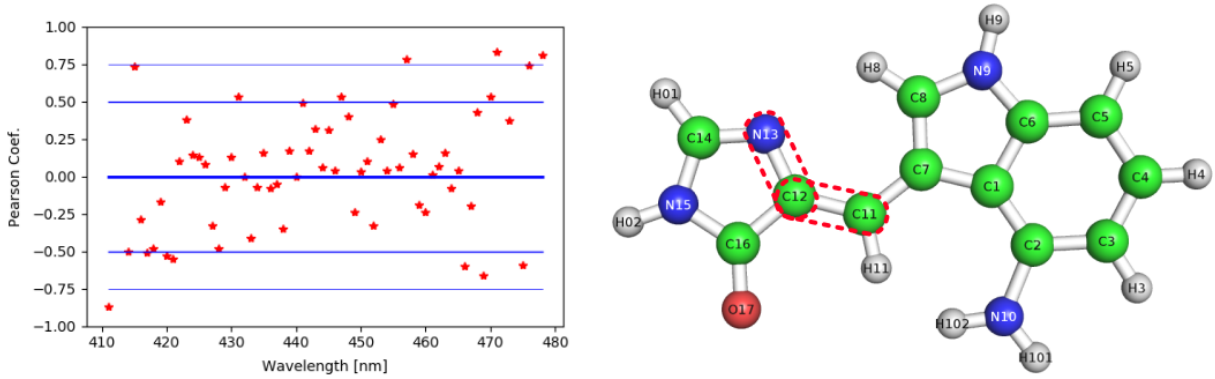

Figure S5 (cont.): Pearson correlation analysis of angle "N13–C12–C11".

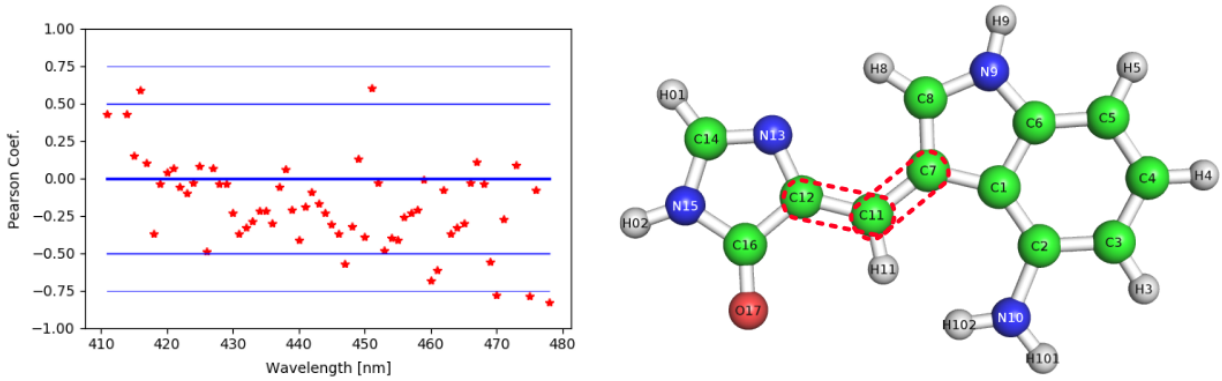

Figure S5 (cont.): Pearson correlation analysis of angle "C12–C11–C7".

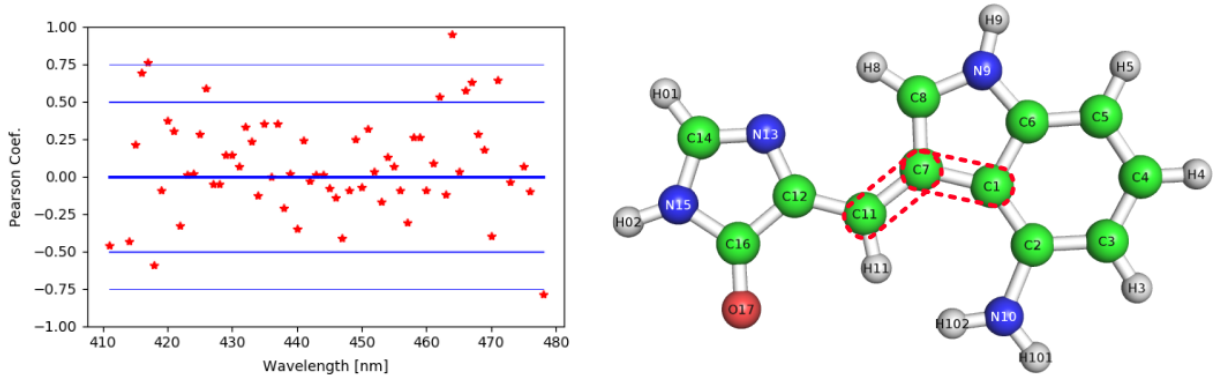

Figure S5 (cont.): Pearson correlation analysis of angle "C11–C7–C1".

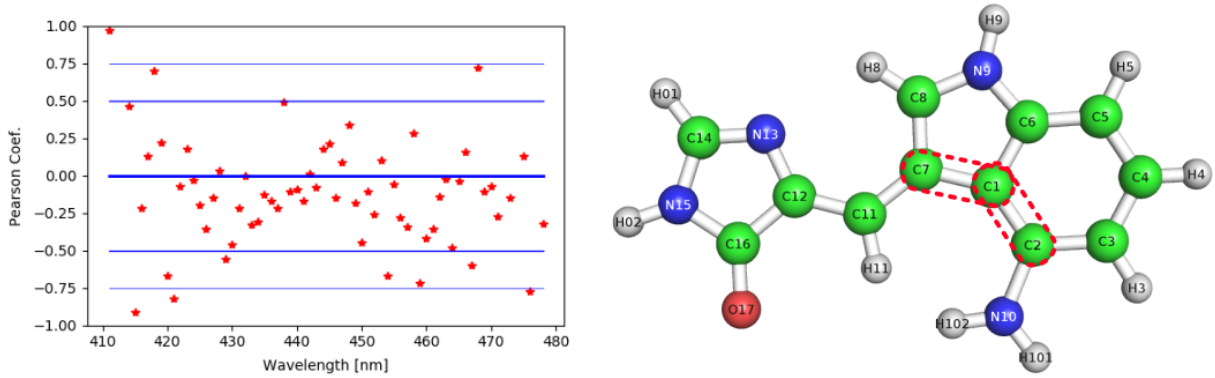

Figure S5 (cont.): Pearson correlation analysis of angle "C7–C1–C2".

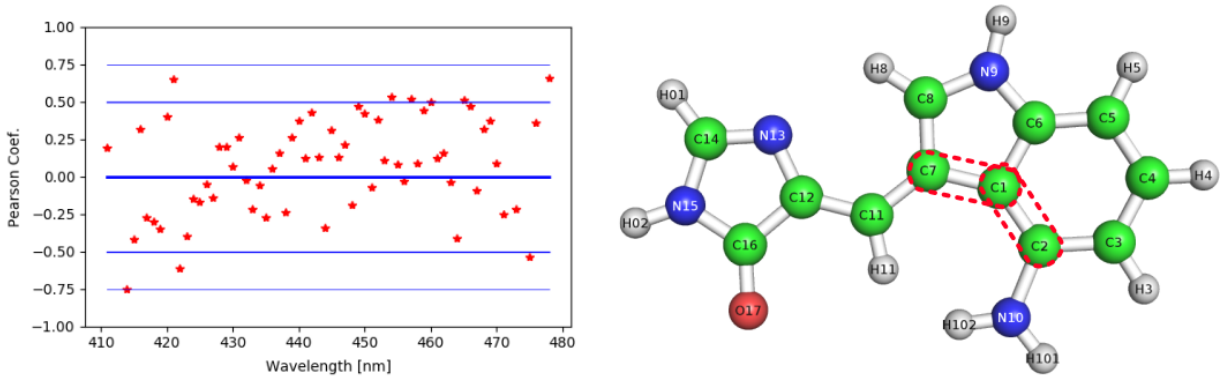

Figure S5 (cont.): Pearson correlation analysis of angle "C7–C1–C2".

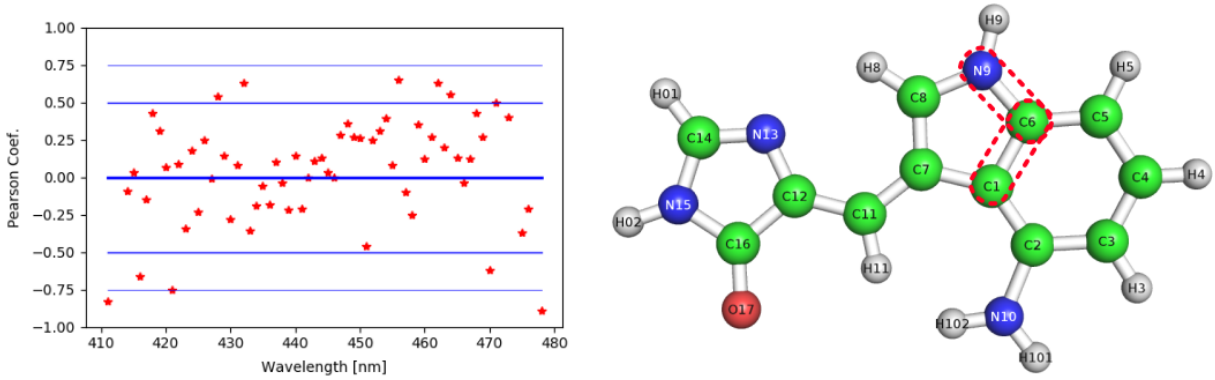

Figure S5 (cont.): Pearson correlation analysis of angle "C1–C6–N9".

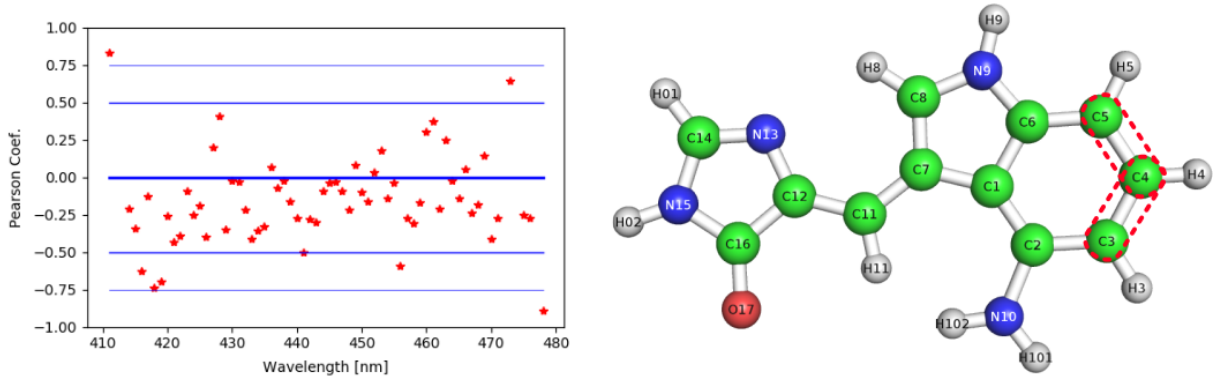

Figure S5 (cont.): Pearson correlation analysis of angle "C3–C4–C5".

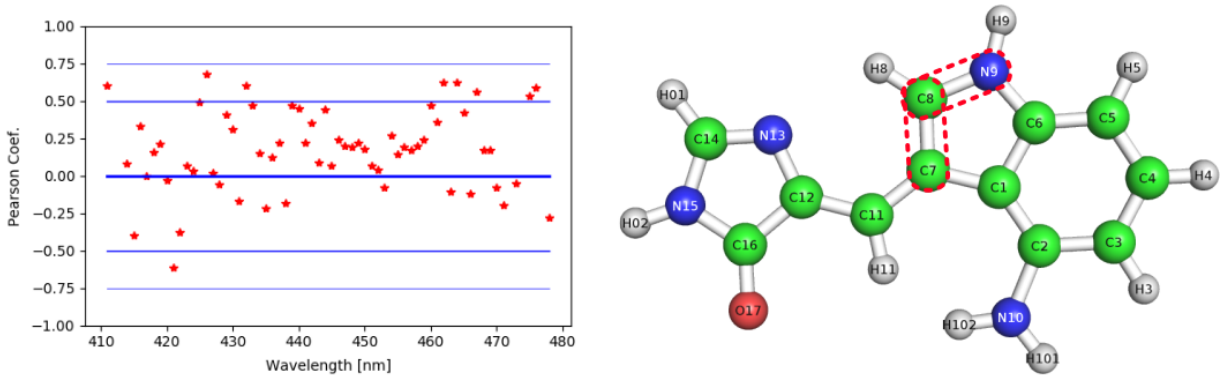

Figure S5 (cont.): Pearson correlation analysis of angle "C7–C8–N9".

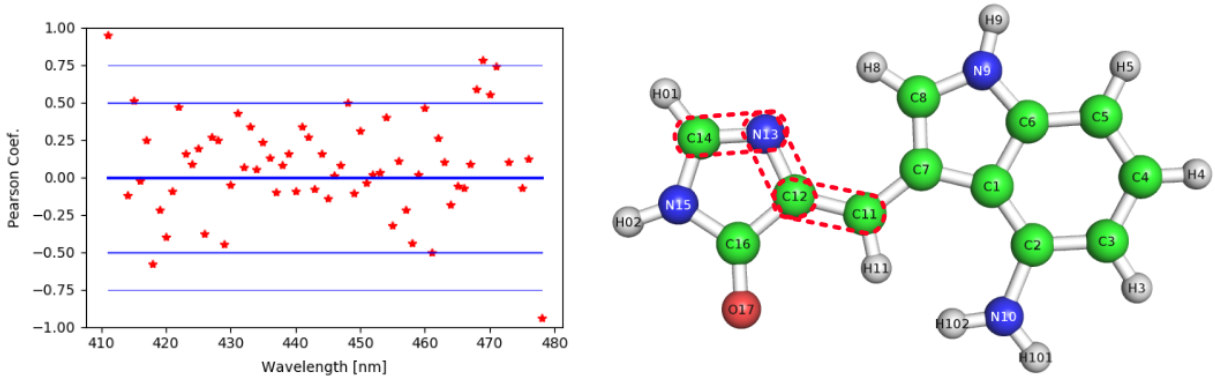

Figure S6: Pearson correlation analysis of dihedral "C14–N13–C12–C11".

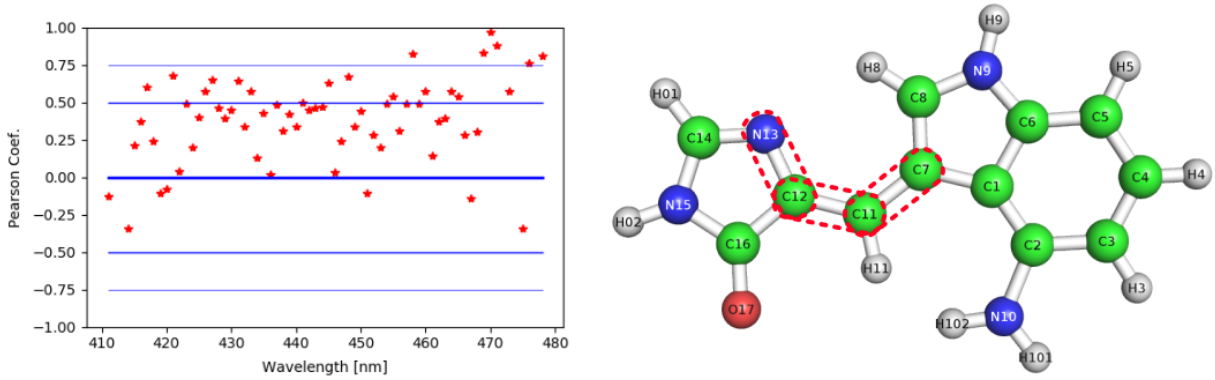

Figure S6 (cont.): Pearson correlation analysis of dihedral "N13–C12–C11–C7".

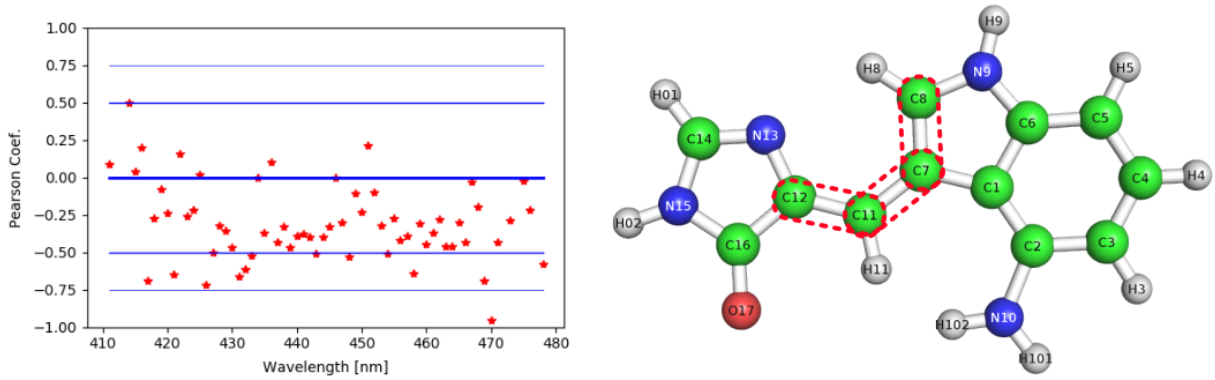

Figure S6 (cont.): Pearson correlation analysis of dihedral "C12–C11–C7–C8".

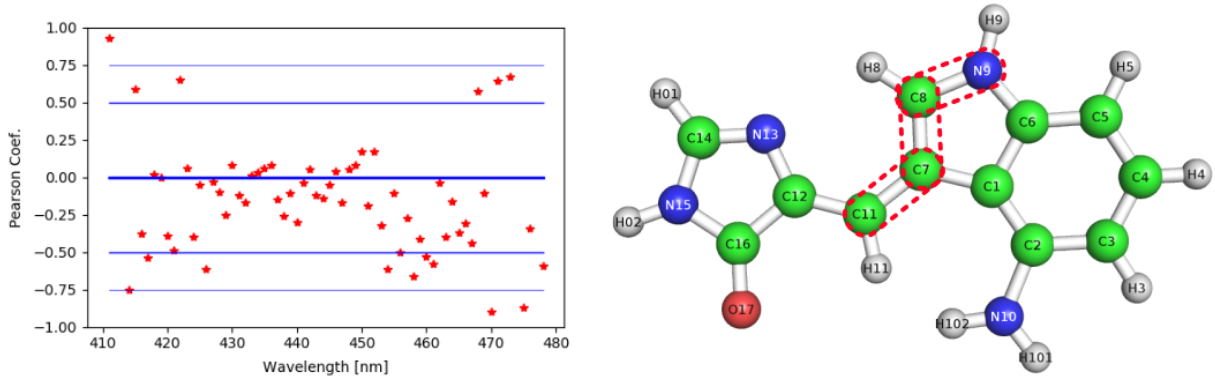

Figure S6 (cont.): Pearson correlation analysis of dihedral "C11–C7–C8–N9".

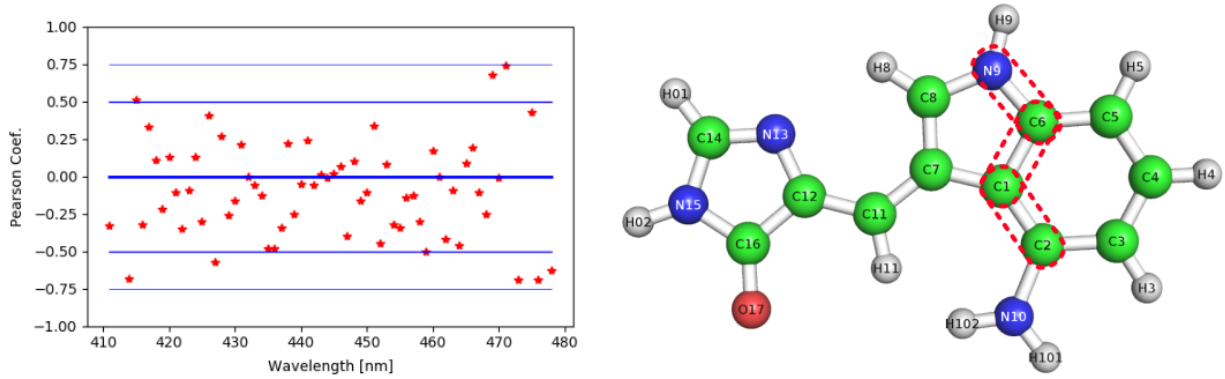

Figure S6 (cont.): Pearson correlation analysis of dihedral "N9–C6–C1–C2".

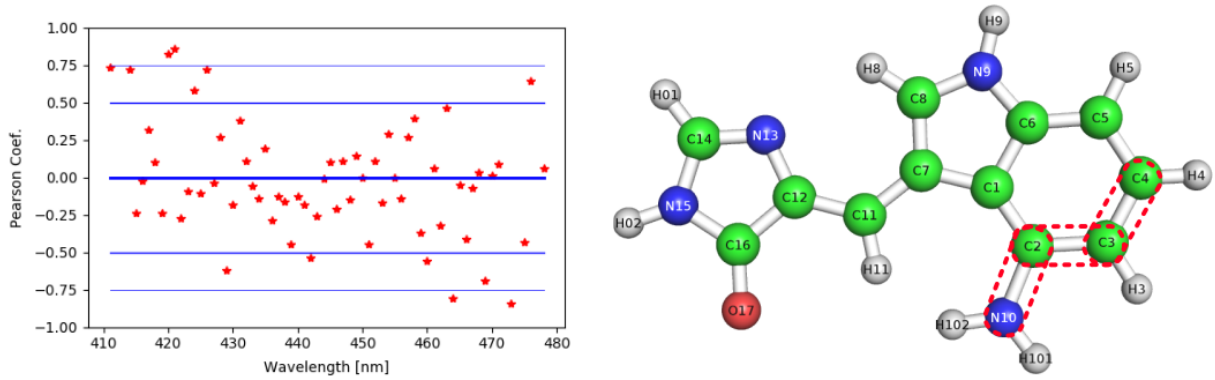

Figure S6 (cont.): Pearson correlation analysis of dihedral "N10–C2–C3–C4".

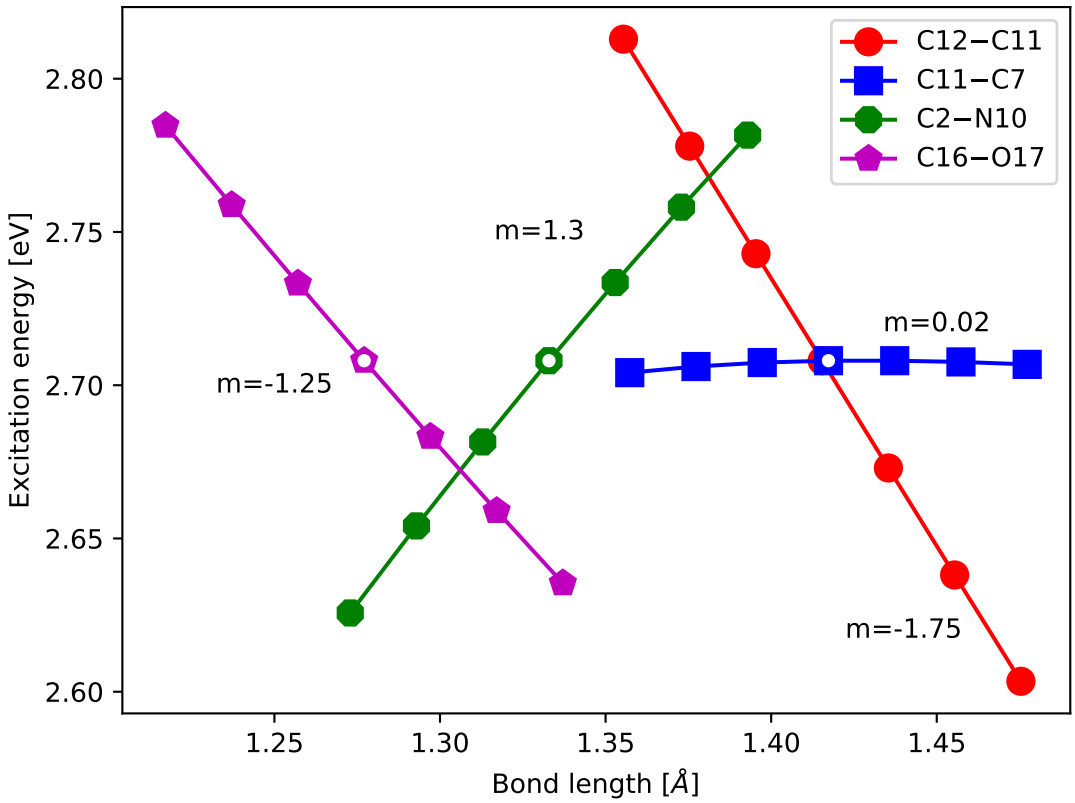

Figure S7: Excitation energies with respect to bond lengths. Computed at the CAM-B3LYP/6-31G+(d) level of theory. Equilibrium bond lengths are showed with white circles on the markers. The m values are the slope of lines.

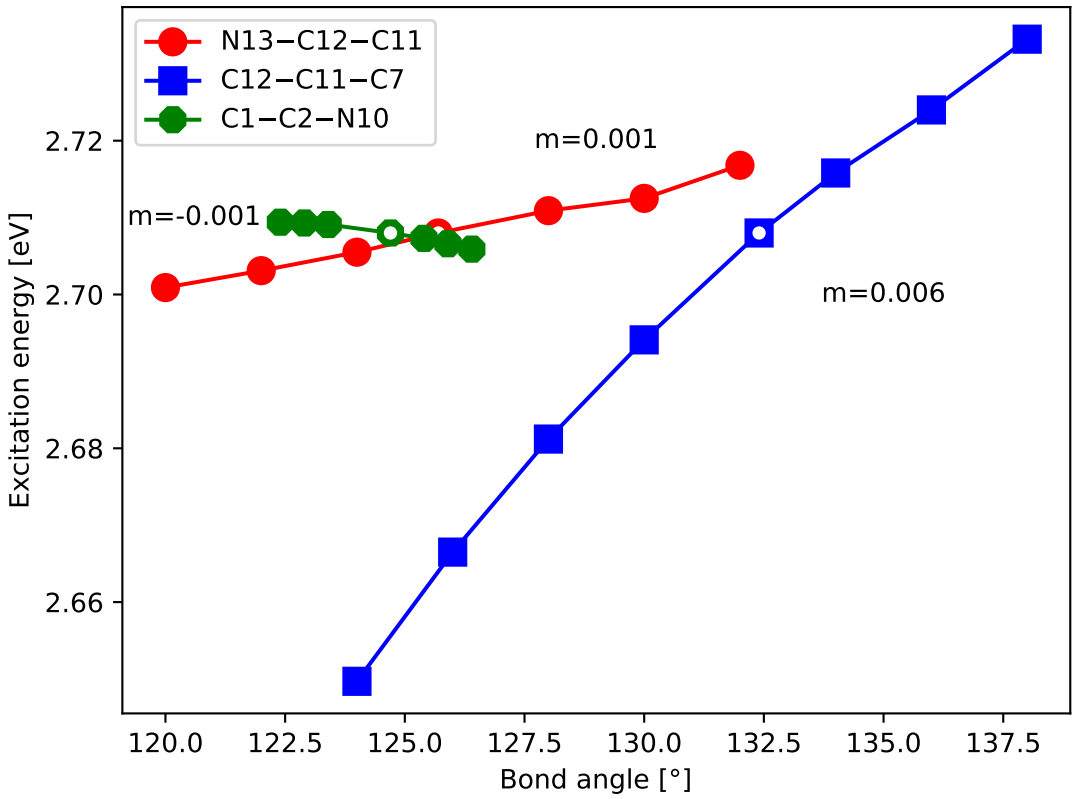

Figure S8: Excitation energies with respect to bond angles. Computed at the CAM-B3LYP/6-31G+(d) level of theory. Equilibrium bond lengths are showed with white circles on the markers. The m values are the slope of lines.

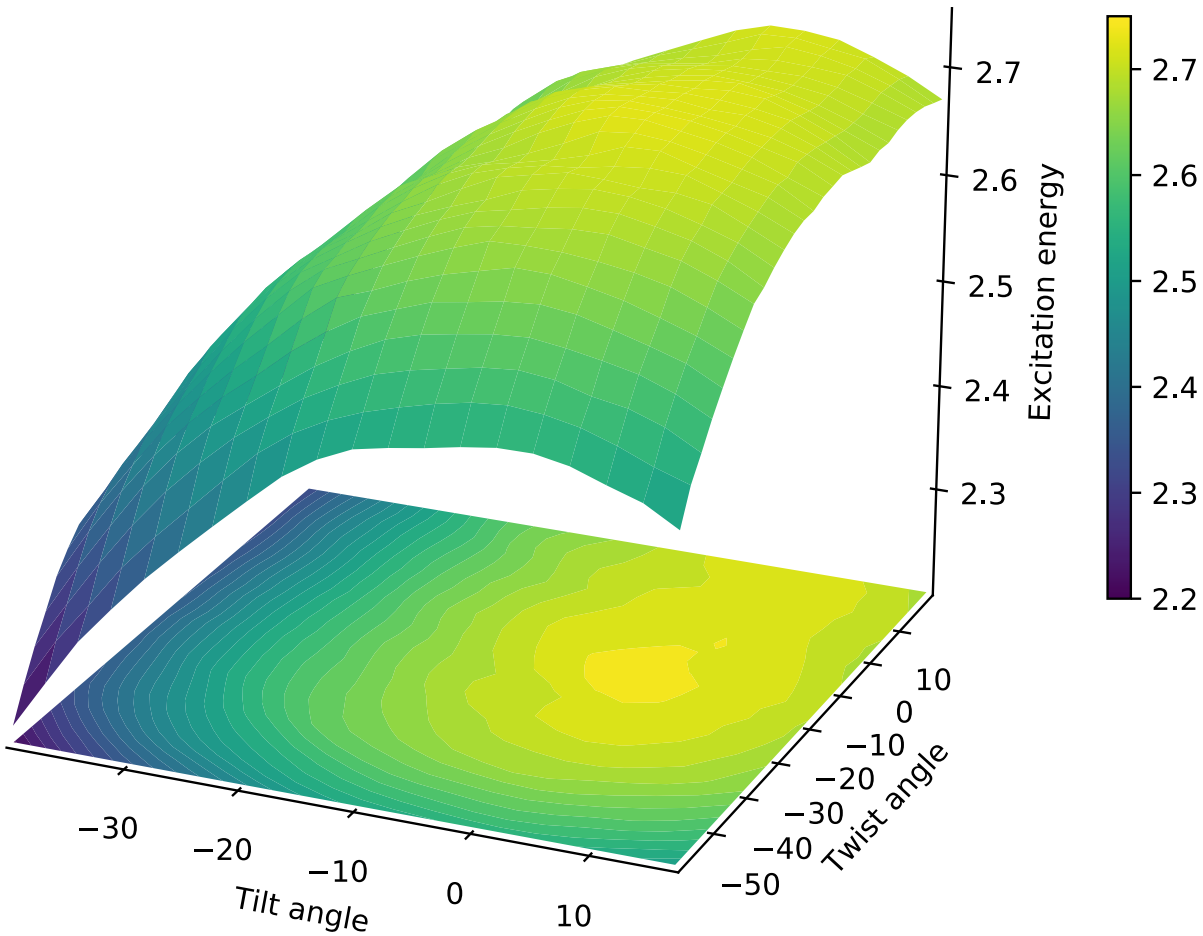

Figure S9: Excitation energies with respect to tilt (θ) and twist (ϕ) dihedrals. Computed at the CAM-B3LYP/6-31G+(d) level of theory.

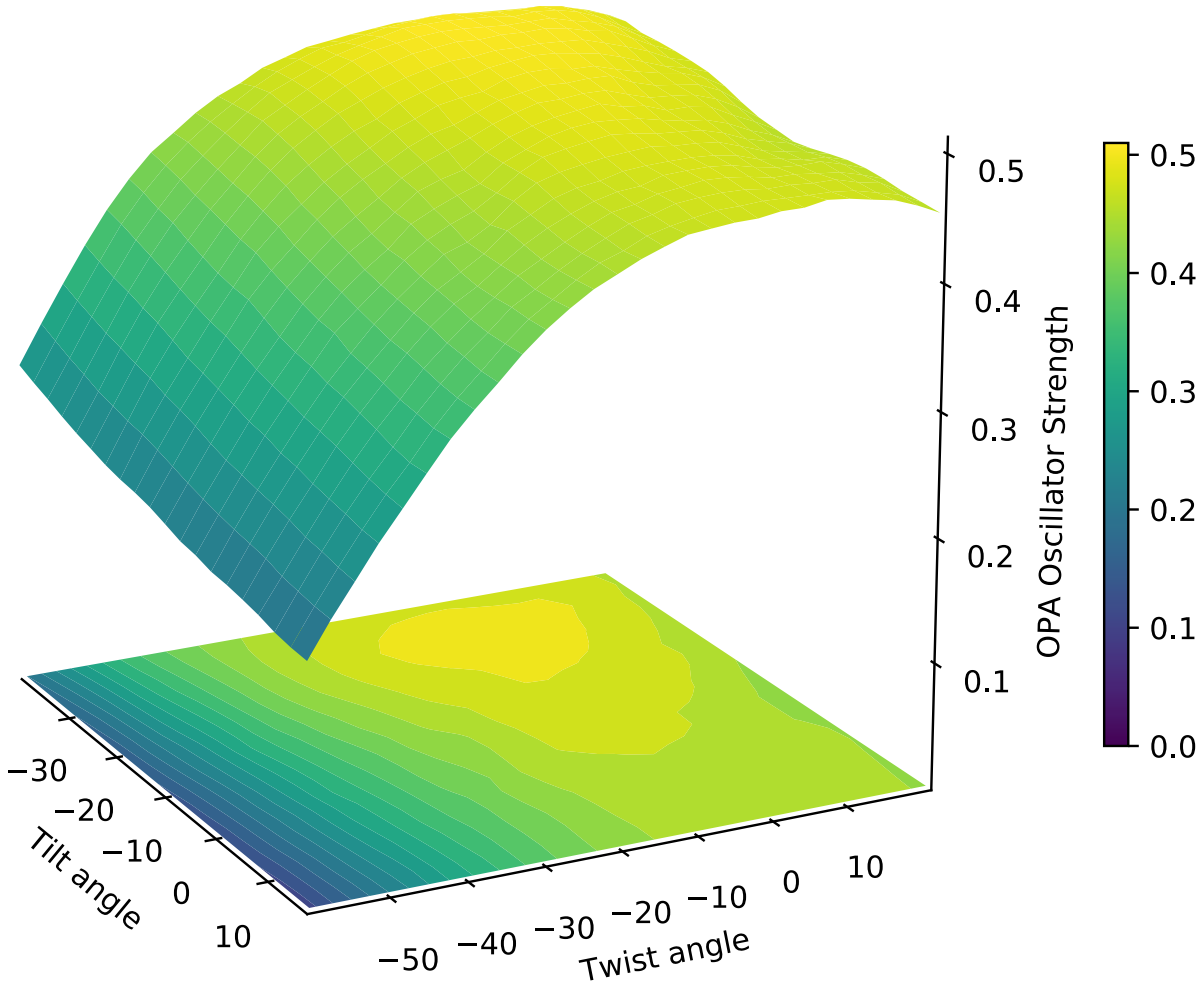

Figure S10: Oscillator strengths of excited states with respect to tilt (θ) and twist (ϕ) dihedrals. Computed at the CAM-B3LYP/6-31G+(d) level of theory.

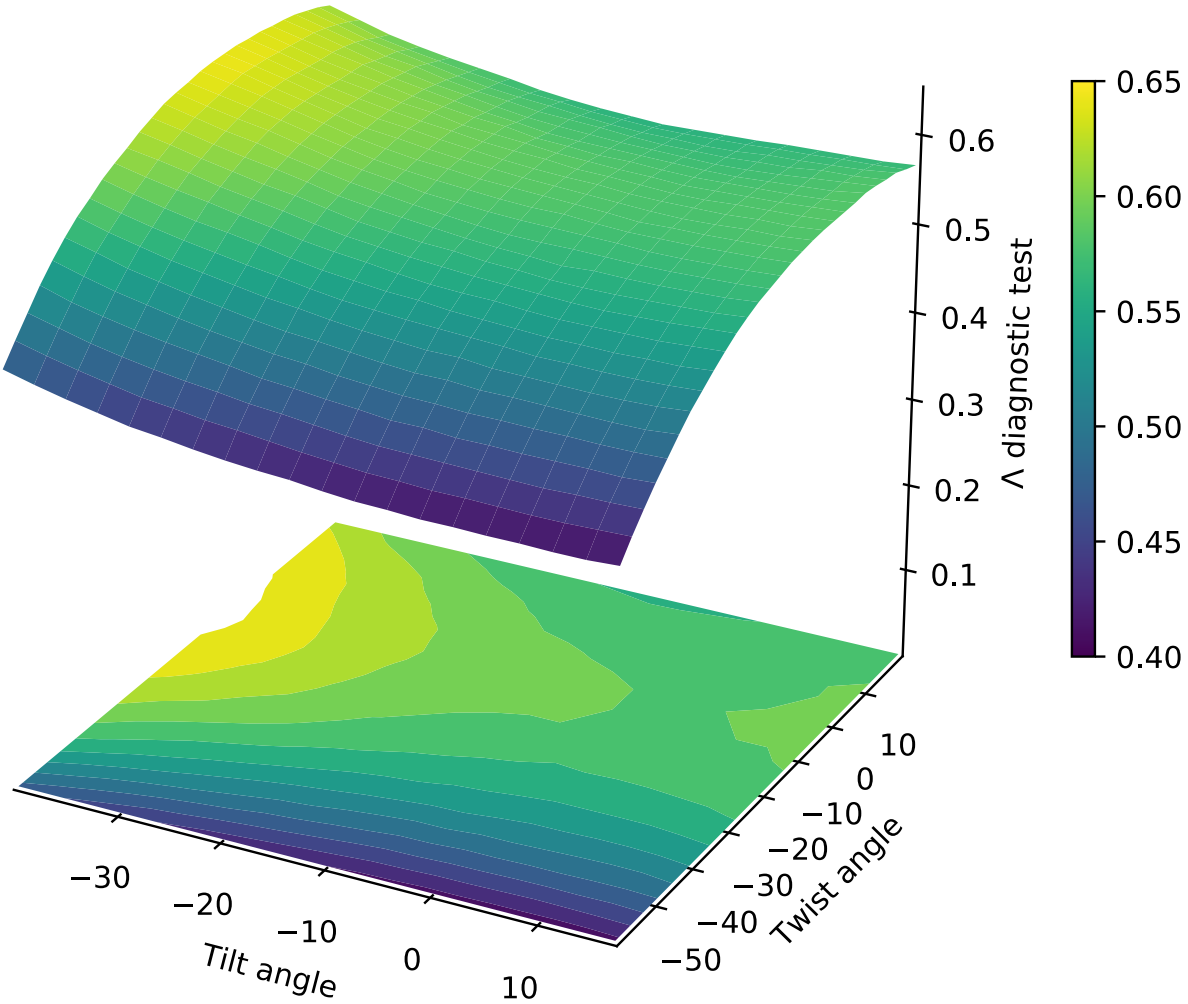

Figure S11: Lambda diagnostic evaluations of excited states with respect to tilt (θ) and twist (ϕ) dihedrals. Computed at the CAM-B3LYP/6-31G+(d) level of theory.

References

(1) Bayly, C. I.; Cieplak, P.; Cornell, W.; Kollman, P. A. *J. Phys. Chem.* **1993**, *97*, 10269–10280.

(2) Humphrey, W.; Dalke, A.; Schulten, K. *Journal of Molecular Graphics* **1996**, *14*, 33–38.